McStas 1.12b - a New Release of the Flexible Neutron Ray-tracing Package

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Abstract

Since release 1.0 in october 1998, the McStas[1],[2] neutron ray-tracing simulation package has been hosted at Risø in strong collaboration the ILL in Grenoble, University of Copenhagen and the PSI.

During its lifetime, McStas has evolved to become the world leading software in the area of neutron scattering simulations for instrument design, optimisation, virtual experiments[3][4][5] and science.

This poster draws an outline of the McStas software package and recent achievements.

McStas Facts

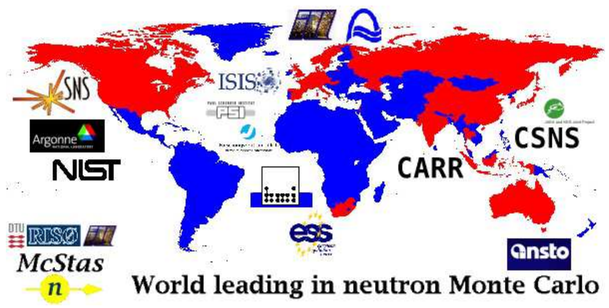

Figure 1: *McStas world dissemination. We are represented in the red-colured parts of the world*

- McStas first official release in October 1998 (v. 1.0)
- McStas is now (June 2010) at release 1.12b
- Next major release is 2.0, expected early 2011
- McStas has 136 components in cathegories of
- Continuous and pulsed neutron sources
- Neutron optics, including polarized equipment
- Sample components for incoherent scattering, powders, single crystals (structural and magnetic), phonons, liquids, small angle scattering
- Monitor components
- McStas now includes support for polarised neutrons
- McStas includes 66 example instruments
- McStas has complete documentation and tutorial material, all included
- McStas is free, open source software (GNU Public License version 2.0)
- McStas includes valuable user contributions
- McStas is used at all major neutron scattering facilities
- McStas is platform independent, Ubuntu GNU/Linux 9.10 & 10.4., Windows XP & Vista & 7, Mac OS X 10.3-10.6, in 32 and 64 bit are fully supported
- McStas features easy to use parallelisation methods for multi-core machines, clusters and grids
- Installation is straightforward on all the platforms, but we provide VMware and Knoppix based solutions for users who want that. Ready to run - NO installation!

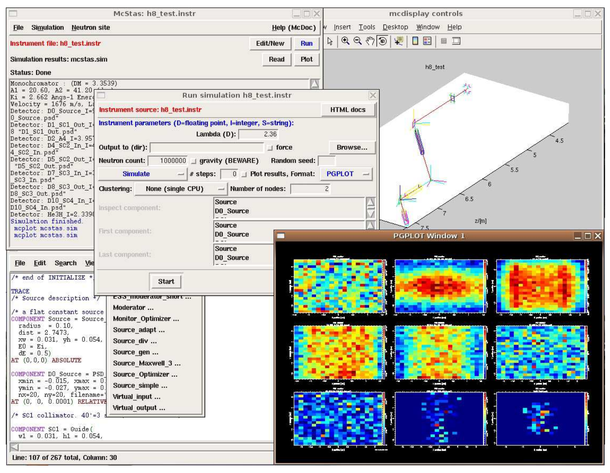

Figure 2: *Overview in graphics of features and possibilities of the McStas simulation package*

McStas for Instrument design and optimisation

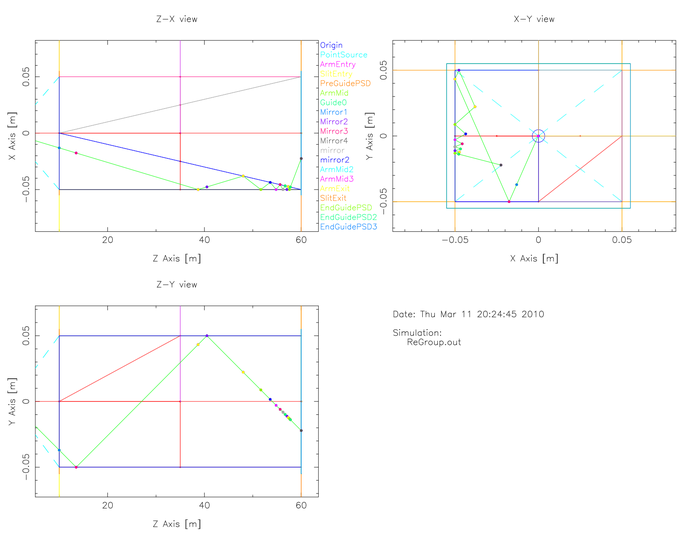

Figure 3: Building comp assemblies [6] *Visualisation of single neutron ray travelling through single-mirror guide with inserted wedge mirrors.*

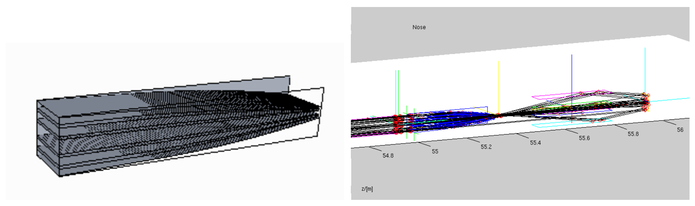

Figure 4: Courtesy E. Farhi, K. Andersen, A. Wiedenmann (ILL) - multi-angle SANS realized by focusing optics and monochromators.

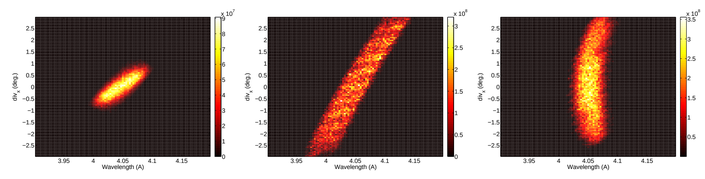

Figure 5: Cold TAS optimisation from [7] *Correlations between wavelength and horizontal divergence at the sample position, in arbitrary units. a) the baseline design, b) the manually optimized solution, c) the final elliptical solution.*

McStas for Virtual Experiments

IN6 @ ILL, liquid Ge

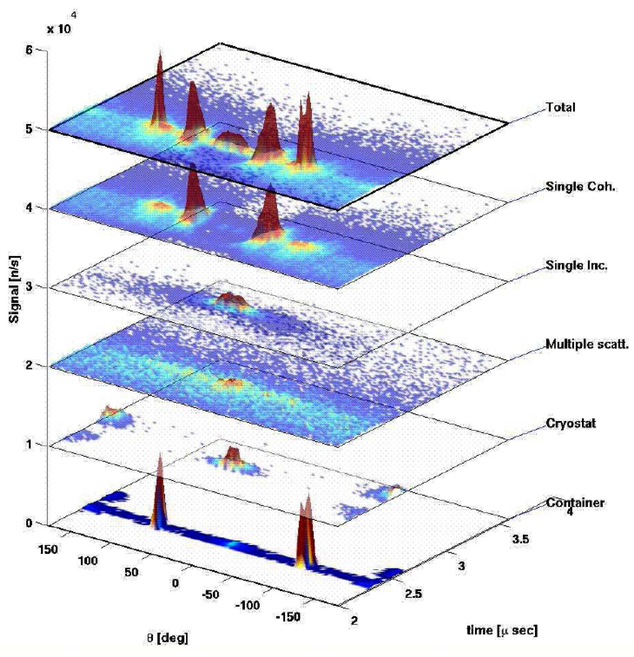

Figure 6: From [4] *Example virtual experiment, luiquid germanium at ILL IN6 TOF machine. Full detector signal and its composition: Single coherent scattering, Single incoherent scattering, Multiple scattering, cryostat and container contributions.*

DMC @ PSI, $Na_2Ca_3Al_2F_{14}$

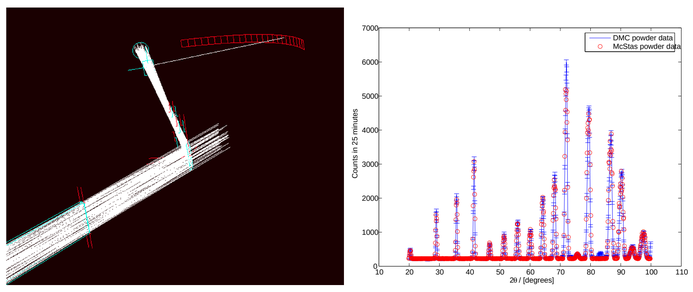

Figure 7: From [3] *DMC @ PSI instrument simulated using McStas. Left: 3D-display of the instrument. Right: Powder lines from $Na_2Ca_3Al_2F_{14}$. Comparison between virtual experiment and diffractometer data.*

Polarised neutrons, spin-echo

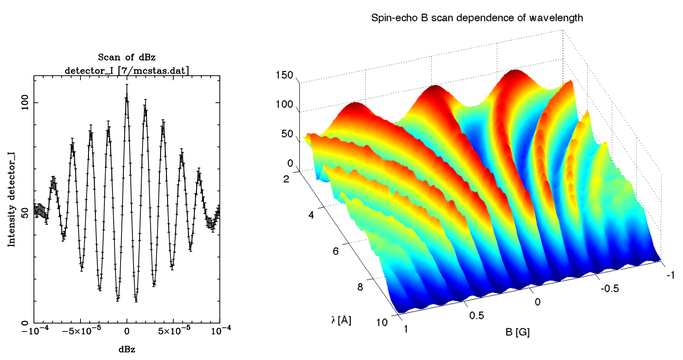

Figure 8: *Virtual spin-echo data from a future first reference about polarised neutron scattering using McStas.*

Highlight themes, McStas 2.x series

- New Components
  - 4-dimensional S(Q,w) - first approach from a analytical expressions
  - Single_crystal like component with possibilties of local strain, size and orientation distributions filling the gap to PowderN.
  - New lens components; focusing lenses and refractive lenses
  - Polarisation-oriented samples; Single crystal and powder with magnetic order, spin-flip amplitudes, spin wave component
  - Improved, more physical monochromator comps (possibly “old” contributions Monochromator_reflect Monochromator_crystallite by Lucia Alianelli)
- Polarisation, magnetic fields
  - Magnetic field calculations initiated from McStas (e.g. ala V. Hugouvieux thesis work - Freefem call in INITIALIZE %{%})
  - All components with support for polarized beams
  - New Polarisation example instruments
  - Read-in tables of precomputed B coordinates (ANSYS, Freefem, ...)
- Package standardization
  - Uniform parameter naming for the different component classes; Sources, Samples, Monitors, Guides as specified in the new `NOMENCLATURE` definition in the `lib/`
  - The Obsolete class of components will be emptied, porting functionality in the few cases where this is not available in another component. Components will go to the Obsolete class again through development in the McStas 2.x series.
  - We will ensure proper use of PROP_DT and intersection routines in all comps, to ensure that gravitation and Larmor precession etc. works for *all* components.
  - Supplementing the Test_Incoherent instrument, we will develop other test instruments for intercomparison of similar components. Examples: Test_Fermi; Test_Sources; Test_Guides; Test_Monochromators.
  - During the 2.x series, *all* McStas components will have at least one test condition in the instrument examples.
  - During the 2.x series, *all* McStas example instruments will be seperated in *frontend* and *backend* instrument, allowing easy studies of instrument performance, say at the guide of a different neutron source. This mechanism is connected to the %include keyword, i.e.: ILL_H142_IN12=ILL_H142+templateTAS, ILL_H15_IN6=ILL_H15+templateTOF
  - A new test mechanism has been defined: All example instruments have an McDoc %example line in the header that tells the mcrun –test command what results to expect from this instrument. The test mechanism takes the calculated I_ERR on given monitors into account.
  - All components will be ensured to fully work with MPI
- Documentation
  - New release of the manual and component manual to reflect the standardization work etc.
- Metalanguage and runtime code
  - New grammar(s) for ’Metacomponents’ or ’Multicomponents’ :
    - ARRAY positions=filename COMPONENT MyComp = Comp()
    - GROUP should jump to first member if SCATTERED (allows for multiple scattering, many-mirror setups etc.)
    - Component initiated SPLIT (Transmission/Reflection)
  - Support for zlib packaging of files. Will allow storing in e.g. zipped format for big event files and $S(\vec{Q},\omega)$ tables
- Tools and platform support
  - New GUI (Python,wXwidgets,matplotlib/gnuplot considered)
  - Web-enabled, but secure GUI (Ajax or equivalent)
  - Port of McStas to interesting new hardware/possibilities:
    - Playstation 3 (Cell processor with 1 CPU, 7 GPU)
    - Nvidia GPU’s via CUDA
    - McStas@Home (put your machine in the ESS simulation GRID)
  - New mcresplot-like tool
  - Optimizer based on SWARM / Genetic algorithm
  - Scan over ’strings’

    `filename=whatever.dat;whatever2.dat;whatever3.dat -N 3`
  - Scans in more than one dimension
  - N-dimensional output in case of scans (or Volume data - e.g. PSD versus scanned parameters)

References

[1] K. Lefmann and K. Nielsen, *McStas, a General Software Package for Neutron Ray-tracing Simulations*, Neutron News 10, 20, (1999).

[2] McStas project website at http://www.mcstas.org

[3] P. Willendrup et al.: *Validation of a realistic powder sample using data from DMC at PSI*, ICNS 2005 proceedings.

[4] Hugouvieux V, Farhi E, Johnson MR, et al.: *Structure and dynamics of l-Ge: Neutron scattering experiments and ab initio molecular dynamics simulations"*, PRB 75 (2007) 104208

[5] K. Lefmann et al., *Virtual experiments - the ultimate aim of neutron ray-tracing simulations*, Journal of Neutron Research 16, 97-111 (2008)

[6] P. Willendrup et al., *Using McStas for modelling complex optics, using simple building bricks*, NIMA (in press doi:10.1016/j.nima.2010.06.212)

[7] K. Lefmann et al., *Optimal shape of a cold-neutron triple-axis spectrometer*, NIMA, (in press doi:10.1016/j.nima.2010.06.273)

Keywords: McStas, Monte Carlo sim., Software, Neutrons, Instruments
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